ABSTRACT

Background: Periodontitis is currently diagnosed almost entirely on gross clinical manifestations. Also potential biomarkers are generally studied individually and rarely in small numbers. This may explain why the predictive value of potential biomarkers studied to date has not been sufficient for routine clinical use. Infrared spectroscopy measures the total contents of a sample and should prove a powerful diagnostic and prognostic tool for periodontal diseases.

Aim: The aim of the study was to employ IR spectroscopy to characterize saliva from healthy, chronic periodontitis, aggressive periodontitis and to determine specific spectral signatures that clearly demarcates healthy and diseased tissues in chronic and aggressive periodontitis patients.

Materials and Methods: Unstimulated whole saliva samples were obtained from 66 subjects (22 chronic periodontitis, 22 aggressive periodontitis and 22 healthy subjects). 50 µl saliva sample was dried on BaF window in a vacuum desiccator and IR spectra were recorded using a FTIR spectrometer. Band integrations of relative components of each spectrum were calculated using Opus software. Linear discriminant analysis were used to correlate observed spectral differences of saliva from aggressive periodontitis and chronic periodontitis and control samples. ANOVA test and Dunnett t – test were performed to find whether the mean difference of IR spectra was significant among the three groups.

Results: Linear discriminant analysis revealed that the overall accuracy for the classification of saliva samples as control or aggressive periodontitis was 73.9% for the training set and 67.1% for the validation set. The overall accuracy for the classification of saliva samples as control or chronic periodontitis was 67.7% for the training set and 56.7% for the validation set. The mean difference of IR spectra was

increased for wavelengths 1087 cm^{-1} (symmetric Po_2^- stretching vibrations of phosphodiester groups), 1240 cm^{-1} (asymmetric Po_2^- stretching vibrations of phosphodiester groups), 1542 cm^{-1} (amide II band), 1652 cm^{-1} (amide I band), 1740 cm^{-1} (lipid ester), 3050 cm^{-1} (amide B band) and 3290 cm^{-1} (amide A) in aggressive and chronic periodontitis when compared to controls. ANOVA test revealed that the mean difference of IR spectra between control and periodontitis groups was significant for wavelengths 1087 cm^{-1}, 1240 cm^{-1} and 1652 cm^{-1} at the 0.01 level ($p<0.01$) and also significant for wavelength 1740 cm^{-1} at the 0.05 level ($p<0.05$). There was a significant increase in the mean IR spectra in aggressive periodontitis when compared to chronic periodontitis for wavelengths 1087 cm^{-1}, 1240 cm^{-1} and 1652 cm^{-1} and 1740 cm^{-1}, which corresponds to symmetric Po_2^- stretching vibrations of phosphodiester groups in DNA, asymmetric Po_2^- stretching vibrations of phosphodiester groups in DNA, amide I band and lipid ester respectively. Dunnett t – test revealed that the mean difference of IR spectra was significant for wavelengths 1087 cm^{-1}, 1240 cm^{-1}, 1652 cm^{-1} at the 0.05 level ($p<0.05$) when aggressive periodontitis and chronic periodontitis were compared with healthy controls and also significant for wavelength 1740 cm^{-1} at the 0.05 level ($p<0.05$), when aggressive periodontitis was compared with healthy controls but not significant when chronic periodontitis was compared with healthy controls.

Conclusion: Thus, it was possible to clearly demarcate the periodontitis patients and healthy subjects and also the diagnosis of aggressive periodontitis and chronic periodontitis can be established by doing IR analysis of saliva. Disease specific molecular alterations occur in the saliva and the molecular signatures of saliva in aggressive and chronic periodontitis can be determined by IR spectroscopic analysis. Thus IR spectroscopy can be used as a non-invasive, rapid, reagent-free, cost

effective method for the diagnosis of aggressive periodontitis and chronic periodontitis by analysing saliva sample. IR spectroscopy can also be used as a tool to differentiate between aggressive and chronic periodontitis thus helping in the diagnosis.

Key words: Saliva; infra red spectroscopy; molecular signatures; chronic periodontitis; aggressive periodontitis.